=> file reg
FILE 'REGISTRY' ENTERED AT 09:07:31 ON 29 AUG 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 27 AUG 2003 HIGHEST RN 574700-05-3 DICTIONARY FILE UPDATES: 27 AUG 2003 HIGHEST RN 574700-05-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> file hcapl
FILE 'HCAPLUS' ENTERED AT 09:07:41 ON 29 AUG 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 29 Aug 2003 VOL 139 ISS 10 FILE LAST UPDATED: 28 Aug 2003 (20030828/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que L4 STR

```
1 c c 3
1 c c 3
6 c 4 c 0H 13
6 c 7 c 68
9 c c 11
14 NH2

14 NH2
```

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L6 438 SEA FILE=REGISTRY SSS FUL L4 L7 232 SEA FILE=HCAPLUS ABB=ON L6

L8 7 SEA FILE=HCAPLUS ABB=ON L7 AND (HAIR OR KERAT?)

=> d 18 1-7 all hitstr

7 CA references with ulitity

```
L8 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2003 ACS on STN
```

AN 2002:675838 HCAPLUS

DN 137:216934

- TI Preparation of fused cyclic succinimide compounds and analogs thereof, as modulators of nuclear hormone receptor function
- IN Salvati, Mark E.; Attar, Ricardo M.; Gottardis, Marco M.; Balog, James A.;
 Pickering, Dacia A.; Martinez, Rogelio L.; Sun, Chongqing
- PA Bristol-Myers Squibb Company, USA
- SO PCT Int. Appl., 331 pp. CODEN: PIXXD2

DT Patent

LA English

- IC ICM A61K031-495
- CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom)) Section cross-reference(s): 1, 2, 27

FAN.CNT 1

		-																	
	PATENT NO.				KIND DATE					APPLICATION NO.					DATE				
										-									
PI	WO 2002067939			A1 20020906			WO 2002-US5302						20020220						
		W:	ΑE,	ΑG,	AL,	ΑM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,	
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,	
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	ΝZ,	OM,	PH,	
			PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	TZ,	
			ÜΑ,	UG,	US,	UZ,	VN,	YU,	ZA,	ZM,	ZW,	AM,	ΑZ,	BY,	KG,	KZ,	MD,	RU,	
			ТJ,																
		RW:	GH.	GM.	KE.	LS.	MW.	MZ.	SD.	STL	SZ.	TZ.	UG.	2M -	7.W .	ΑТ.	BE.	CH-	

CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG PRAI US 2001-271672P P 20010227
OS MARPAT 137:216934
GI

AΒ Title compds. I [G = (un)substituted cycloalkenyl, aryl or heterocyclo (mono or polycyclic); Z1 and Z2 independently = O, S, NH or substituted amine; L = bond, substituted alkyl chain, NH, substituted amine; A1 and A2 independently = CR1 or N when Y = J-J'-J'' where J = (CR1R1')n with n =0-3, J' = bond, carbonyl, CR1R1', R2P:O, R2P:S, etc., and W =CR1R1'-CR1R1', CR3:CR3', (un)substituted cycloalkyl, etc.; or when Y is absent A1 and A2 independently = CR1R1' or NR1; or when Y is absent A1, A2 and W together form -NR1-N:N-; Q1 and Q2 independently = H, (un) substituted alkyl, alkenyl, cycloalkyl, etc.; R1 and R1' independently = H, (un) substituted alkyl, alkenyl, cycloalkyl, cycloalkenyl, amino, halo, CN, etc.; R2 = (un)substituted alkyl, cycloalkyl, cycloalkenyl, heterocyclo, aryl, arylalkyl, etc.; R3 and R3' independently = H, (un) substituted alkyl, alkenyl, CN, halo, nitro, amino, etc.] are prepd. and methods of using such compds. in the treatment of nuclear hormone receptor-assocd. conditions, and pharmaceutical compns. contg. such compds are disclosed. Thus, II was prepd. by cyclocondensation of (3a.alpha., 4.beta., 8.beta., 8a.alpha.) -4,5,6,7,8,8a-hexahydro-4,8-etheno-1Hcyclohepta[c]furan-1,3(3aH)dione (prepn. given) with 3-(trifluoromethyl)aniline. Combinatorial methods of prepg. compds. of formula I are also provided. As modulators of nuclear hormone receptor function, the use of I as potential anticancer agents and for treatment of immune disorders is claimed (no data).

ST isoindoledione prepn nuclear hormone receptor function antitumor immune disorder; succinimide fused cyclic prepn cancer antitumor immune disorder; combinatorial library isoindoledione prepn nuclear hormone receptor disorder

IT Prostate gland, neoplasm

(adenocarcinoma; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function)

ELHILO 10/0493

IT Drugs
(appetion isoind)

IT Muscle, disoind)

IT Prostate (carcin modula)

IT Menopause (disordisoind)

IT Menopause (disordisoind)

IT Menopause (disordisoind)

IT Wegina

IT

ΙT

IT

IT

(appetite stimulants; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function)

isoindolediones as modulators of nuclear hormone receptor function Muscle, disease

(atrophy, inhibition of; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function) Prostate gland, neoplasm

(carcinoma; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function)

opause
(disorder, hot flash; prepn. of substituted fused cyclic
isoindolediones as modulators of nuclear hormone receptor function)

(disorder; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function)

(dryness; treatment of; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function)

IT Heart, disease
 (failure; prepn. of substituted fused cyclic isoindolediones as
 modulators of nuclear hormone receptor function)

Hair preparations
 (growth inhibitors; prepn. of substituted fused cyclic isoindolediones
 as modulators of nuclear hormone receptor function)

IT Hair preparations
(growth stimulants; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function)

IT Reproductive tract, disease (hypogonadism, treatment of; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function)

IT Abortion
 (induced; prepn. of substituted fused cyclic isoindolediones as
 modulators of nuclear hormone receptor function)

IT Parturition
 (inducing; prepn. of substituted fused cyclic isoindolediones as
 modulators of nuclear hormone receptor function)

Uterus, neoplasm
 (leiomyoma; prepn. of substituted fused cyclic isoindolediones as
 modulators of nuclear hormone receptor function)

Alopecia
(male pattern; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function)

(polycystic, treatment of; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function) Combinatorial library

(prepn. of combinatorial libraries of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function). IT Alzheimer's disease Angiogenesis Angiogenesis inhibitors Anorexia Anti-Alzheimer's agents Anti-inflammatory agents Anticholesteremic agents Antidiabetic agents Antipsychotics Antitumor agents Cachexia Cardiovascular agents Contraceptives Heart, disease Human Inflammation Mammary gland, neoplasm Neoplasm Osteoporosis (prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function) IT Mental disorder (psychosis; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function) TΤ Androgens RL: BSU (Biological study, unclassified); BIOL (Biological study) (replacement therapy, treatment of decreased testosterone levels in men; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function) TT Appetite (stimulants; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function) IT Spermatogenesis (suppressing; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function) IT Osteoporosis (therapeutic agents; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function) IT Dopamine receptors RL: BSU (Biological study, unclassified); BIOL (Biological study) (treatment of disorders mediated by; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function) IT Androgen receptors Estrogen receptors RL: BSU (Biological study, unclassified); BIOL (Biological study) (treatment of tumor cells contg.; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function) ΙT Acne Autoimmune disease Drug dependence Hirsutism Seborrhea (treatment of; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function) 2746-19-2P IT 944-40-1P 944-41-2P 7124-34-7P 14166-28-0P

73252-09-2P

115419-41-5P 249259-68-5P

29577-71-7P

17812-27-0P

```
455279-73-9P
                   455279-74-0P
                                  455279-75-1P
    RL: CRT (Combinatorial reactant); RCT (Reactant); SPN (Synthetic
    preparation); CMBI (Combinatorial study); PREP (Preparation); RACT
     (Reactant or reagent)
        (intermediate; prepn. of substituted fused cyclic isoindolediones as
       modulators of nuclear hormone receptor function)
IT
    610-93-5P
                931-22-6P
                            17402-82-3P, Benzo[b]thiophen-3-amine
    32896-90-5P
                  56587-27-0P
                                65399-05-5P
                                              67081-02-1P
                                                             73306-79-3P
    99864-95-6P
                  155172-19-3P
                                 406224-21-3P
                                                 455279-76-2P
                   455279-79-5P
                                  455279-80-8P
                                                  455279-81-9P
    455279-78-4P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (intermediate; prepn. of substituted fused cyclic isoindolediones as
       modulators of nuclear hormone receptor function)
ΙT
                                                 85-42-7, 1,2-
    63-74-1, 4-Aminosulfonylaniline 83-55-6
    Cyclohexanedicarboxylic anhydride
                                        85-43-8
                                                 91-59-8, 2-Naphthalenamine
    93-05-0, 4-(N,N-Diethylamino)aniline
                                           94-09-7
                                                      95-03-4,
    5-Chloro-2-methoxyaniline
                                95-55-6, 2-Aminophenol
                                                         95-64-7,
                          95-74-9, 3-Chloro-4-methylaniline
    3,4-Dimethylaniline
                                                              95-76-1,
                                    98-16-8, 3-(Trifluoromethyl)aniline
    3,4-Dichloroaniline 96-74-2
    99-03-6, 3-Acetylaniline
                              99-09-2, 3-Nitroaniline
                                                        99-31-0 99-88-7,
    4-Isopropylaniline 100-01-6, 4-Nitroaniline, reactions
                                                                104-10-9,
    4-(2-Hydroxyethyl)aniline 104-96-1, 4-Methylthioaniline
                                                                106-40-1,
    4-Bromoaniline 106-47-8, 4-Chloroaniline, reactions
                                                            108-44-1,
    3-Methylaniline, reactions 108-69-0, 3,5-Dimethylaniline
                                                                  117-40-8
    118-46-7
               118-92-3, 2-Aminobenzoic acid 119-32-4, 4-Methyl-3-
    nitroaniline
                  119-34-6, 3-Nitro-4-hydroxyaniline 121-50-6,
    2-Chloro-5-(trifluoromethyl)aniline 121-87-9, 2-Chloro-4-nitroaniline
    129-64-6, cis-5-Norbornene-endo-2,3-dicarboxylic anhydride 132-32-1
              134-32-7, 1-Aminonaphthalene 137-07-5, 2-Mercaptoaniline
    137-17-7, 2,4,5-Trimethylaniline 150-13-0, 4-Aminobenzoic acid
    153-78-6, 2-Fluorenylamine 156-43-4, 4-Ethoxyaniline
                                                              320-51-4,
    4-Chloro-3-(trifluoromethyl)aniline 364-13-6 364-76-1,
    4-Fluoro-3-nitroaniline 367-21-5, 4-Fluoro-3-chloroaniline 2,4,5-Trifluoroaniline 368-53-6 371-40-4, 4-Fluoroaniline
                                                                    367 - 34 - 0,
                                                                     372-16-7.
                                    372-19-0, 3-Fluoroaniline
    4-(Trifluoromethylthio)aniline
                         393-11-3, 4-Nitro-3-(trifluoromethyl)aniline
    3,5-Difluoroaniline
    393-36-2
              438-32-4
                          452-69-7, 4-Fluoro-3-methylaniline 452-84-6,
    2-Fluoro-5-methylaniline
                              455-14-1, 4-Trifluoromethylaniline
                                                                     462-08-8,
    3-Pyridinamine 504-24-5, 4-Aminopyridine 504-29-0, 2-Pyridinamine
    533-30-2, 6-Benzothiazolamine 535-52-4, 2-Fluoro-5-
    (trifluoromethyl)aniline
                              540-37-4, 4-Iodoaniline
                                                         551-93-9
                                                                     578-66-5,
    8-Aminoquinoline
                      580-15-4, 6-Quinolinamine
                                                   580-19-8, 7-Quinolinamine
    587-02-0, 3-Ethylaniline
                              589-16-2, 4-Ethylaniline
                                                           611-05-2,
    3-Methyl-4-nitroaniline
                              611-34-7, 5-Quinolinamine
                                                           618 - 87 - 1,
    3,5-Dinitroaniline 626-01-7, 3-Iodoaniline
                                                    626-40-4,
    3,5-Dibromoaniline
                         626-43-7, 3,5-Dichloroaniline
                                                          634-91-3,
    3,4,5-Trichloroaniline
                             635-22-3, 4-Chloro-3-nitroaniline
    2,4,5-Trichloroaniline
                             654-70-6
                                        713-62-2
                                                   720-98-9
                                                               722-92-9
               776-34-1, 1-Amino-4-nitronaphthalene
                                                      784-57-6
                                                                  825-41-2,
    3-Chloro-4-nitroaniline
                              873-74-5, 4-Aminobenzonitrile
                                                              1008-95-3
    1125-60-6, 5-Isoquinolinamine 1198-64-7
                                                1484-26-0, 3-Benzyloxyaniline
    1535-73-5, 3-(Trifluoromethoxy) aniline
                                            1544-85-0
                                                         1603-40-3,
    2-Amino-3-methylpyridine
                               1687-53-2, 2-Methoxy-5-aminophenol
                                                                     1824-81-3,
                               1877-77-6, 3-(Hydroxymethyl)aniline
    2-Amino-6-methylpyridine
    2051-53-8, 2-Methyl-5-isopropylaniline 2217-40-5
                                                         2243-61-0,
    1,4-Naphthalenediamine 2243-62-1, 1,5-Naphthalenediamine 2246-44-8
               2307-00-8 2357-47-3, 4-Fluoro-3-(trifluoromethyl)aniline
    2298-07-9
```

```
2359-60-6, 4-(1-Piperidinyl)aniline
                                     2524-67-6
                                                 2696-84-6,
4-(n-Propyl)aniline 2834-90-4 3096-57-9, 2-Amino-9H-fluoren-9-one
3102-87-2, 1,4-Diamino-2,3,5,6-tetramethylbenzene
                                                   3230-35-1
                                                               3325-11-9,
1H-Benzotriazol-5-amine 3425-89-6
                                    3470-54-0
                                                 3535-75-9
                                                             3544-25-0,
4-Cyanomethylaniline
                      3638-73-1, 2,5-Dibromoaniline
                                                      3682-14-2
3862-73-5, 2,3,4-Trifluoroaniline
                                   3863-11-4, 3,4-Difluoroaniline
3886-70-2
           4106-66-5, 3-Dibenzofuranamine
                                           4469-78-7
                                                       4518-10-9
4684-12-2, 4-Chloro-1-naphthalenamine 4730-93-2 4760-53-6
                                                               4993-96-8
5192-03-0, 1H-Indol-5-amine 5307-14-2, 2-Nitro-4-aminoaniline
5333-84-6
           5345-54-0, 3-Chloro-4-methoxyaniline
                                                  5348-42-5,
1,2-Diamino-4,5-dichlorobenzene 5369-16-4, 3-Isopropylaniline
5369-19-7, 3-(tert-Butyl)aniline
                                 5438-24-4
                                              5443-16-3
5470-49-5, 4-Methylsulfonylaniline
                                    5650-01-1
                                                5834-17-3
                                                            5930-28-9,
3,5-Dichloro-4-hydroxyaniline
                               6004-79-1
                                           6313-37-7
                                                       6315-89-5,
3,4-Dimethoxyaniline 6344-62-3
                                  6358-07-2, 2-Amino-4-chloro-5-
              6373-46-2, 4-Benzyloxyaniline
nitrophenol
                                             6376-14-3
                                                         6623-41-2,
2-Amino-4,5-dimethylphenol
                            6628-04-2
                                        6933-10-4, 4-Bromo-3-
methylaniline
                6942-37-6
                           6967-12-0, 1H-Indazol-6-amine
                                                           7149-75-9,
3-Methyl-4-chloroaniline
                          7365-74-4
                                      7418-43-1
                                                  10420-89-0
                                                               13171-61-4
                         14268-66-7, 1,3-Benzodioxol-5-amine
13207-66-4
            13788-70-0
                                                               14415-44-2
14763-20-3, 3-Chlorophenylhydrazine
                                     14806-35-0
                                                  15918-79-3
                                                               16153-81-4
16452-01-0, 4-Methyl-3-methoxyaniline
                                       16712-58-6
                                                    16889-21-7
             17823-38-0
16994-13-1
                         17823-89-1
                                      17824-28-1
                                                   18978-78-4
             19335-11-6, 1H-Indazol-5-amine
19063-57-1
                                             19438-60-9
                                                          19840-99-4
19947-75-2
             20012-63-9, 2-Benzyloxyaniline
                                             20191-74-6
                                                          20870-91-1
20925-27-3
             20929-46-8
                         21116-13-2
                                      21402-26-6, 4-Bromo-3-chloroaniline
21901-40-6
             22013-33-8
                         22246-07-7
                                      22865-62-9, 4-Methylsulfinylaniline
23031-78-9, 1,2-Benzisothiazol-3-amine
                                        23679-72-3
                                                     24313-88-0.
3,4,5-Trimethoxyaniline 24327-08-0, endo-Bicyclo[2.2.2]-5-octene-2,3-
dicarboxylic anhydride
                        24425-40-9
                                     24447-28-7
                                                  25392-18-1
                                                               25464-96-4
25900-61-2
             26093-31-2
                         26210-75-3
                                      27492-84-8
                                                   28094-04-4
28657-75-2
             28786-85-8 30202-92-7
                                      31951-12-9, 4-(tert-Butyl)-3-
nitroaniline
              33630-94-3
                           34762-56-6
                                        35212-85-2, Methyl-3-
aminobenzothiophene-2-carboxylate 35944-64-0, 3-Iodo-4-methylaniline
37559-33-4
            40444-36-8
                        42984-96-3
                                      46047-18-1 50432-01-4,
                            50670-64-9, 5-Amino-2-methylbenzonitrile
2,6-Diphenyl-4-aminophenol
51123-09-2
            51387-92-9
                        51606-73-6
                                      51606-74-7 53312-81-5,
5-Amino-2-fluorobenzonitrile
                              53324-08-6
                                          53518-15-3
                                                        54396-44-0,
2-Methyl-3-(trifluoromethyl)aniline
                                     55048-24-3
                                                  55396-63-9 56354-98-4
56587-29-2
             56746-19-1, 4-Bromo-2,6-diethylaniline
                                                     57334-19-7
57805-85-3
             58721-76-9
                        58728-64-6
RL: CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial
study); RACT (Reactant or reagent)
   (prepn. of substituted fused cyclic isoindolediones as modulators of
   nuclear hormone receptor function)
62261-58-9
            62368-29-0
                        65079-19-8 65382-95-8
                                                   67567-26-4,
4-Bromo-2,6-difluoroaniline
                             70654-85-2
                                          74159-77-6
                                                       89586-07-2
89793-82-8
            90111-40-3
                         90721-35-0
                                      91391-90-1
                                                   91973-40-9
97051-69-9
            99865-96-0
                         100710-39-2
                                       116481-67-5
                                                     121180-51-6
123458-65-1
             134018-53-4, 3-Benzofuranamine
                                              134050-76-3
                                                            134514-34-4
134992-40-8
             135050-44-1, 3-Chloro-4-iodoaniline
                                                   143173-93-7
147752-39-4
             155338-68-4
                           156901-61-0
                                         157252-24-9
                                                       163733-96-8.
3,4,5-Trifluoroaniline
                       175135-08-7
                                                    175205-10-4
                                      175135-55-4
175277-91-5
             177995-39-0
                                         195046-42-5
                           195046-32-3
                                                       198077-72-4
207974-07-0
             218929-90-9
                           243666-11-7
                                         243977-15-3
                                                       267648-18-0
314272-29-2
             404827-78-7
                           455279~82-0
                                         455279-83-1
                                                       455279-84-2
455279-85-3
             455279-86-4 455279-87-5
                                         455279-88-6
                                                       455279-89-7
455279-92-2
             455279-93-3
                           455279-94-4
                                         455279-95-5
                                                       455279-96-6
```

ΙT

455279-98-8

455279-97-7

```
455280-02-1
                   455280-03-2
                                 455280-04-3
                                               455280-05-4
                                                             455280-06-5
     455280-07-6
                   455280-08-7
                                 455280-09-8
     RL: CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial
     study); RACT (Reactant or reagent)
        (prepn. of substituted fused cyclic isoindolediones as modulators of
        nuclear hormone receptor function)
IT
     57319-65-0P
     RL: CRT (Combinatorial reactant); RCT (Reactant); SPN (Synthetic
    preparation); CMBI (Combinatorial study); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of substituted fused cyclic isoindolediones as modulators of
        nuclear hormone receptor function)
IT
     71-43-2, Benzene, reactions
                                   89-40-7, 4-Nitrophthalimide
                                                                  108-31-6.
    Maleic anhydride, reactions 544-25-2, Cycloheptatriene
                                                                 592-57-4,
     1,3-Cyclohexadiene
                         616-02-4, Citraconic anhydride
                                                           765-46-8,
     Spiro[2.4]hepta-4,6-diene 825-54-7, 1-Phenylcyclopentene
                                                                   930-30-3,
                           1614-12-6, 1-Aminobenzotriazole
     2-Cyclopenten-1-one
                                                             2758-18-1,
     3-Methyl-2-cyclopenten-1-one
                                   2931-32-0
                                                3853-88-1
                                                            4054-38-0,
     1,3-Cycloheptadiene
                           5418-51-9, 2-Hydroxy-5-nitropyridine
                                                                  6318-55-4
                                           19763-90-7, 3,4-
     17793-95-2, cis-1,2-Dihydrocatechol
    Dichlorophenylhydrazine hydrochloride
                                             28620-12-4, 6-Nitro-2-
    benzothiazolinone
                        36216-80-5, 3-Amino-1,2-benzisoxazole
                                                                 51447-09-7
     54781-19-0, 2-(Trimethylsilyloxy)cyclohexa-1,3-diene
                                                            157701-72-9,
     2-Fluoro-4-nitrobenzaldehyde
                                   198821-79-3
                                                  455279-90-0
                                                                 455279-91-1
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of substituted fused cyclic isoindolediones as modulators of
        nuclear hormone receptor function)
ΙT
     455271-95-1P
    RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic
    preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); USES (Uses)
        (target compd.; prepn. and crystal structure of substituted fused
        cyclic isoindolediones as modulators of nuclear hormone receptor
        function)
TΤ
    74807-08-2P
    RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); RCT
     (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL
     (Biological study); CMBI (Combinatorial study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
        (target compd.; prepn. of combinatorial libraries of substituted fused
        cyclic isoindolediones as modulators of nuclear hormone receptor
        function)
    2015-58-9P
                               15247-36-6P
                  4697-05-6P
                                             19077-67-9P
                                                           19849-14-0P
    26234-46-8P
                  26491-17-8P
                                 43069-64-3P
                                               54962-32-2P
                                                             55099-10-0P
    55099-11-1P
                   55680-87-0P
                                 66318-77-2P
                                               66428-17-9P
                                                             66428-21-5P
     66823-85-6P
                   72657-50-2P
                                 72657-51-3P
                                               74944-59-5P
                                                             89074-15-7P
    89104-84-7P
                  116755-71-6P
                                  131317-28-7P
                                                 132445-68-2P
                                                                146962-96-1P
    168251-89-6P
                    197162-90-6P
                                   201947-27-5P
                                                  217490-18-1P
                                                                 217490-19-2P
    217490-20-5P
                    253865-26-8P
                                   277749-69-6P
                                                  295364-52-2P
                                                                 297742-64-4P
    298682-50-5P
                    299422-77-8P
                                   300818-81-9P
                                                  300818-83-1P
                                                                 308841-90-9P
    312713-26-1P
                    329736-39-2P
                                   329736-49-4P
                                                  346405-87-6P
                                                                 353524-22-8P
    354808-35-8P
                    357387-66-7P
                                   374108-43-7P
                                                  431077-19-9P
                                                                 455272-32-9P
    455272-33-0P
                    455272-34-1P
                                                                 455272-38-5P
                                   455272-36-3P
                                                  455272-37-4P
    455272-40-9P
                    455272-41-0P
                                   455272-42-1P
                                                  455272-45-4P
                                                                 455272-47-6P
    455272-49-8P
                    455272-50-1P
                                  455272-51-2P
                                                  455272-52-3P
                                                                 455272-54-5P
    455272-55-6P
                    455272-57-8P
                                   455272-59-0P
                                                  455272-62-5P
                                                                 455272-63-6P
    455272-65-8P
                    455272-66-9P
                                   455272-67-0P
                                                  455272-68-1P
                                                                 455272-69-2P
```

455279-99-9

455280-00-9

455280-01-0

```
455272-75-0P
455272-71-6P
               455272-72-7P
                               455272-73-8P
                                               455272-74-9P
                                                               455272-81-8P
455272-76-1P
               455272-77-2P
                               455272-79-4P
                                               455272-80-7P
                                                               455272-86-3P
               455272-83-0P
                               455272-84-1P
                                               455272-85-2P
455272-82-9P
                                               455272-91-0P
                                                               455272-92-1P
455272-87-4P
               455272-89-6P
                               455272-90-9P
455272-93-2P
               455272-94-3P
                               455272-95-4P
                                               455272-96-5P
                                                               455272-97-6P
                               455273-01-5P
455272-98-7P
               455273-00-4P
                                               455273-02-6P
                                                               455273-03-7P
                                               455273-07-1P
                                                               455273-08-2P
455273-04-8P
               455273-05-9P
                               455273-06-0P
                                               455273-13-9P
                                                               455273-14-0P
455273-09-3P
               455273-11-7P
                               455273-12-8P
                                                               455273-20-8P
                                               455273-18-4P
455273-15-1P
               455273-16-2P
                               455273-17-3P
                                                               455273-26-4P
455273-21-9P
               455273-22-0P
                               455273-23-1P
                                               455273-24-2P
               455273-28-6P
                               455273-29-7P
                                               455273-30-0P
                                                               455273-31-1P
455273-27-5P
                                               455273-36-6P
                                                               455273-38-8P
455273-32-2P
               455273-33-3P
                               455273-35-5P
               455273-41-3P
                               455273-42-4P
                                               455273-43-5P
                                                               455273-44-6P
455273-39-9P
                                               455273-49-1P
                                                               455273-50-4P
455273-45-7P
               455273-47-9P
                               455273-48-0P
                                                               455273-55-9P
               455273-52-6P
                               455273-53-7P
                                               455273-54-8P
455273-51-5P
455273-57-1P
               455273-58-2P
                               455273-59-3P
                                               455273-60-6P
                                                               455273-61-7P
                                                               455273-67-3P
455273-62-8P
               455273-63-9P
                               455273-64-0P
                                               455273-65-1P
                                               455273-71-9P
                                                               455273-72-0P
455273-68-4P
               455273-69-5P
                               455273-70-8P
                                                               455273-78-6P
455273-73-1P
               455273-74-2P
                               455273-75-3P
                                               455273-77-5P
455273-79-7P
               455273-80-0P
                               455273-81-1P
                                               455273-83-3P
                                                               455273-84-4P
455273-85-5P
               455273-86-6P
                               455273-87-7P
                                               455273-88-8P
                                                               455273-89-9P
455273-90-2P
               455273-91-3P
                               455273-93-5P
                                               455273-96-8P
                                                               455273-99-1P
455274-01-8P
               455274-03-0P
                               455274-05-2P
                                               455274-06-3P
                                                               455274-07-4P
                                               455274-11-0P
                                                               455274-12-1P
455274-08-5P
               455274-09-6P
                               455274-10-9P
455274-13-2P
               455274-14-3P
                               455274-15-4P
                                               455274-16-5P
                                                               455274-17-6P
455274-18-7P
               455274-19-8P
                               455274-20-1P
                                               455274-21-2P
                                                               455274-25-6P
455274-26-7P
               455274-27-8P
                               455274-28-9P
                                               455274-29-0P
                                                               455274-30-3P
455274-32-5P
               455274-33-6P
                               455274-34-7P
                                               455274-35-8P
                                                               455274-36-9P
455274-37-0P
               455274-38-1P
                               455274-40-5P
                                               455274-41-6P
                                                               455274-42-7P
455274-43-8P
               455274-44-9P
                               455274-45-0P
                                               455274-46-1P
                                                               455274-48-3P
               455274-50-7P
                               455274-51-8P
                                               455274-52-9P
                                                               455274-53-0P
455274-49-4P
455274-54-1P
               455274-55-2P
                               455274-56-3P
                                               455274-57-4P
```

RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of combinatorial libraries of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function)

```
IT
     455274-58-5P
                     455274-60-9P
                                    455274-61-0P
                                                    455274-62-1P
                                                                    455274-63-2P
     455274-64-3P
                     455274-65-4P
                                    455274-66-5P
                                                    455274-67-6P
                                                                    455274-68-7P
     455274-69-8P
                     455274-70-1P
                                    455274-71-2P
                                                    455274-72-3P
                                                                    455274-73-4P
     455274-74-5P
                    455274-75-6P
                                    455274-77-8P
                                                    455274-78-9P
                                                                    455274-79-0P
     455274-80-3P
                    455274-81-4P
                                    455274-82-5P
                                                    455274-83-6P
                                                                    455274-84-7P
     455274-85-8P
                    455274-87-0P
                                    455274-88-1P
                                                    455274-89-2P
                                                                    455274-90-5P
     455274-91-6P
                    455274-92-7P
                                    455274-93-8P
                                                    455274-94-9P
                                                                    455274-95-0P
     455274-96-1P
                                    455274-99-4P
                                                                    455275-01-1P
                                                    455275-00-0P
                     455274-98-3P
     455275-02-2P
                     455275-03-3P
                                    455275-04-4P
                                                    455275-05-5P
                                                                    455275-07-7P
     455275-08-8P
                     455275-09-9P
                                    455275-10-2P
                                                    455275-11-3P
                                                                    455275-12-4P
     455275-13-5P
                     455275-14-6P
                                    455275-15-7P
                                                    455275-16-8P
                                                                    455275-18-0P
     455275-19-1P
                     455275-20-4P
                                    455275-21-5P
                                                    455275-22-6P
                                                                    455275-23-7P
     455275-24-8P
                     455275-25-9P
                                    455275-26-0P
                                                    455275-27-1P
                                                                    455275-29-3P
     455275-30-6P
                     455275-31-7P
                                    455275-32-8P
                                                    455275-33-9P
                                                                    455275-34-0P
     455275-35-1P
                    455275-36-2P
                                    455275-37-3P
                                                    455275-40-8P
                                                                    455275-41-9P
     455275-42-0P
                     455275-43-1P
                                    455275-44-2P
                                                    455275-45-3P
                                                                    455275-46-4P
     455275-47-5P
                    455275-48-6P
                                    455275-49-7P
                                                    455275-50-0P
                                                                    455275-51-1P
     455275-53-3P
                     455275-54-4P
                                    455275-55-5P
                                                    455275-56-6P
                                                                    455275-57-7P
     455275-58-8P
                     455275-59-9P
                                    455275-60-2P
                                                    455275-61-3P
                                                                    455275-62-4P
     455275-64-6P
                                    455275-66-8P
                                                    455275-67-9P
                                                                    455275-68-0P
                     455275-65-7P
```

```
455275-74-8P
455275-69-1P
               455275-70-4P
                               455275-71-5P
                                               455275-73-7P
455275-75-9P
               455275-76-0P
                               455275-77-1P
                                               455275-78-2P
                                                               455275-79-3P
               455275-82-8P
                               455275-83-9P
                                               455275-84-0P
                                                               455275-85-1P
455275-80-6P
                                                               455275-90-8P
455275-86-2P
               455275-87-3P
                               455275-88-4P
                                               455275-89-5P
455275-91-9P
               455275-93-1P
                               455275-94-2P
                                               455275-95-3P
                                                               455275-96-4P
455275-97-5P
               455275-98-6P
                               455275-99-7P
                                               455276-00-3P
                                                               455276-01-4P
455276-03-6P
               455276-04-7P
                               455276-05-8P
                                               455276-06-9P
                                                               455276-07-0P
455276-08-1P
               455276-09-2P
                               455276-10-5P
                                               455276-12-7P
                                                               455276-13-8P
455276-14-9P
               455276-15-0P
                               455276-16-1P
                                               455276-18-3P
                                                               455276-19-4P
455276-20-7P
               455276-21-8P
                               455276-22-9P
                                               455276-24-1P
                                                               455276-25-2P
455276-26-3P
               455276-27-4P
                               455276-28-5P
                                               455276-30-9P
                                                               455276-32-1P
                                               455276-36-5P
455276-33-2P
               455276-34-3P
                               455276-35-4P
                                                               455276-37-6P
455276-39-8P
               455276-40-1P
                               455276-41-2P
                                               455276-42-3P
                                                               455276-43-4P
                                               455276-47-8P
455276-44-5P
               455276-45-6P
                               455276-46-7P
                                                               455276-48-9P
455276-50-3P
               455276-51-4P
                                               455276-53-6P
                               455276-52-5P
                                                               455276-54-7P
455276-55-8P
               455276-56-9P
                               455276-57-0P
                                               455276-58-1P
                                                               455276-59-2P
455276-60-5P
               455276-61-6P
                               455276-62-7P
                                               455276-64-9P
                                                               455276-65-0P
455276-66-1P
               455276-67-2P
                               455276-68-3P
                                               455276-69-4P
                                                               455276-70-7P
455276-71-8P
               455276-72-9P
                               455276-74-1P
                                               455276-75-2P
                                                               455276-76-3P
455276-77-4P
               455276-78-5P
                               455276-79-6P
                                               455276-80-9P
                                                               455276-81-0P
455276-83-2P
               455276-84-3P
                               455276-85-4P
                                               455276-86-5P
                                                               455276-87-6P
455276-88-7P
               455276-89-8P
                               455276-91-2P
                                               455276-92-3P
                                                               455276-93-4P
               455276-96-7P
                               455276-97-8P
455276-95-6P
                                               455276-98-9P
                                                               455276-99-0P
                               455277-03-9P
455277-00-6P
               455277-02-8P
                                               455277-04-0P
                                                               455277-05-1P
455277-06-2P
               455277-07-3P
                               455277-08-4P
                                               455277-09-5P
                                                               455277-10-8P
455277-11-9P
               455277-12-0P
                               455277-13-1P
                                               455277-14-2P
                                                               455277-15-3P
455277-17-5P
               455277-18-6P
                               455277-19-7P
                                               455277-20-0P
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU
```

RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)

(target compd.; prepn. of combinatorial libraries of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function)

```
455277-21-1P
                     455277-22-2P
                                                    455277-24-4P
TT
                                     455277-23-3P
                                                                    455277-25-5P
                     455277-27-7P
     455277-26-6P
                                     455277-28-8P
                                                    455277-29-9P
                                                                    455277-30-2P
                                     455277-33-5P
     455277-31-3P
                     455277-32-4P
                                                    455277-34-6P
                                                                    455277-35-7P
                     455277-37-9P
     455277-36-8P
                                     455277-38-0P
                                                    455277-39-1P
                                                                    455277-40-4P
     455277-41-5P
                     455277-42-6P
                                     455277-43-7P
                                                    455277-44-8P
                                                                    455277-45-9P
     455277-46-0P
                     455277-47-1P
                                     455277-48-2P
                                                    455277-49-3P
                                                                    455277-50-6P
     455277-51-7P
                     455277-52-8P
                                    .455277-53-9P
                                                    455277-54-0P
                                                                    455277-55-1P
     455277-56-2P
                     455277-57-3P
                                     455277-58-4P
                                                    455277-59-5P
                                                                    455277-60-8P
     455277-61-9P
                     455277-62-0P
                                     455277-63-1P
                                                    455277-65-3P
                                                                    455277-66-4P
     455277-67-5P
                     455277-68-6P
                                     455277-69-7P
                                                    455277-70-0P
                                                                    455277-72-2P
     455277-73-3P
                     455277-74-4P
                                     455277-75-5P
                                                    455277-76-6P
                                                                    455277-77-7P
     455277-78-8P
                                     455277-80-2P
                                                    455277-82-4P
                     455277-79-9P
                                                                    455277-83-5P
                                                    455277-87-9P
     455277-84-6P
                     455277-85-7P
                                     455277-86-8P
                                                                    455277-88-0P
     455277-89-1P
                     455277-90-4P
                                     455277-91-5P
                                                    455277-93-7P
                                                                    455277-94-8P
     455277-95-9P
                     455277-96-0P
                                                    455277-99-3P
                                     455277-97-1P
                                                                    455278-00-9P
     455278-01-0P
                     455278-02-1P
                                     455278-04-3P
                                                    455278-05-4P
                                                                    455278-06-5P
     455278-07-6P
                     455278-08-7P
                                     455278-09-8P
                                                    455278-10-1P
                                                                    455278-11-2P
     455278-13-4P
                     455278-14-5P
                                     455278-15-6P
                                                    455278-16-7P
                                                                    455278-17-8P
     455278-18-9P
                     455278-19-0P
                                     455278-21-4P
                                                    455278-22-5P
                                                                    455278-23-6P
     455278-24-7P
                     455278-25-8P
                                     455278-26-9P
                                                    455278-27-0P
                                                                    455278-29-2P
     455278-30-5P
                     455278-32-7P
                                     455278-33-8P
                                                    455278-34-9P
                                                                    455278-35-0P
     455278-36-1P
                     455278-37-2P
                                     455278-38-3P
                                                    455278-39-4P
                                                                    455278-40-7P
     455278-42-9P
                     455278-44-1P
                                     455278-45-2P
                                                    455278-46-3P
                                                                    455278-47-4P
                                                                    455278-53-2P
     455278-48-5P
                     455278-49-6P
                                     455278-51-0P
                                                    455278-52-1P
     455278-54-3P
                     455278-55-4P
                                     455278-56-5P
                                                    455278-57-6P
                                                                    455278-58-7P
```

ΙT

ΙT

ΙT

IT

```
455278-60-1P
               455278-61-2P
                               455278-62-3P
                                              455278-63-4P
                                                              455278-64-5P
               455278-66-7P
                               455278-67-8P
                                              455278-68-9P
                                                              455278-69-0P
455278-65-6P
                                              455278-73-6P
                                                              455278-74-7P
455278-70-3P
               455278-71-4P
                               455278-72-5P
                                                              455278-81-6P
455278-77-0P
               455278-78-1P
                               455278-79-2P
                                              455278-80-5P
               455278-83-8P
                               455278-84-9P
                                              455278-85-0P
                                                              455278-86-1P
455278-82-7P
                                              455278-90-7P
               455278-88-3P
                               455278-89-4P
                                                              455278-91-8P
455278-87-2P
                               455278-95-2P
                                              455278-96-3P
                                                              455278-97-4P
455278-92-9P
               455278-94-1P
455278-98-5P
               455278-99-6P
                               455279-00-2P
                                              455279-01-3P
                                                              455279-02-4P
455279-03-5P
               455279-04-6P
                               455279-05-7P
                                              455279-06-8P
                                                              455279-07-9P
                               455279-10-4P
                                              455279-11-5P
                                                              455279-12-6P
455279-08-0P
               455279-09-1P
                                                              455279-17-1P
455279-13-7P
               455279-14-8P
                               455279-15-9P
                                              455279-16-0P
               455279-19-3P
                               455279-20-6P
                                              455279-21-7P
                                                              455279-22-8P
455279-18-2P
                               455279-25-1P
                                              455279-26-2P
                                                              455279-27-3P
455279-23-9P
               455279-24-0P
                                                              455279-32-0P
               455279-29-5P
                               455279-30-8P
                                              455279-31-9P
455279-28-4P
               455279-34-2P
                               455279-35-3P
                                              455279-36-4P
                                                              455279-37-5P
455279-33-1P
               455279-39-7P
                               455279-40-0P
                                              455279-41-1P
                                                              455279-42-2P
455279-38-6P
455279-43-3P
               455279-44-4P
                               455279-45-5P
                                              455279-46-6P
                                                              455279-47-7P
455279-48-8P
               455279-49-9P
                               455279-50-2P
                                              455279-51-3P
                                                              455279-52-4P
455279-53-5P
               455279-54-6P
                               455279-55-7P
                                              455279-56-8P
                                                              455279-57-9P
455279-59-1P
               455279-60-4P
                               455279-61-5P
                                              455279-62-6P
                                                              455279-63-7P
455279-64-8P
               455279-65-9P
                               455279-66-0P
                                              455279-67-1P
                                                              455279-68-2P
455279-69-3P
               455279-70-6P
                               455279-71-7P
                                              455279-72-8P
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU
(Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study);
PREP (Preparation); USES (Uses)
   (target compd.; prepn. of combinatorial libraries of substituted fused
   cyclic isoindolediones as modulators of nuclear hormone receptor
   function)
455281-05-7P
               455281-06-8P
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU
(Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study);
PREP (Preparation); USES (Uses)
   (target compd.; prepn. of combinatorial libraries of substituted fused
   cyclic isoindolediones as modulators of nuclear hormone receptor
   function)
455271-60-0P
               455271-65-5P
                               455271-75-7P
                                              455272-01-2P
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
CMBI (Combinatorial study); PREP (Preparation); USES (Uses)
   (target compd.; prepn. of substituted fused cyclic isoindolediones as
   modulators of nuclear hormone receptor function)
455271-77-9P
               455271-79-1P
                               455271-82-6P
                                              455271-87-1P
                                                              455271-93-9P
455272-03-4P
               455272-10-3P
                               455272-22-7P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
   (target compd.; prepn. of substituted fused cyclic isoindolediones as
   modulators of nuclear hormone receptor function)
              455271-53-1P
                              455271-56-4P
66428-19-1P
                                             455271-63-3P
                                                             455271-67-7P
455271-69-9P
               455271-70-2P
                               455271-71-3P
                                              455271-72-4P
                                                              455271-73-5P
455271-74-6P
               455271-76-8P
                               455271-78-0P
                                              455271-80-4P
                                                              455271-81-5P
455271-83-7P
               455271-84-8P
                               455271-86-0P
                                              455271-88-2P
                                                              455271-89-3P
455271-91-7P
               455271-92-8P
                               455271-96-2P
                                              455271-99-5P
                                                              455272-05-6P
455272-07-8P
               455272-08-9P
                               455272-11-4P
                                              455272-12-5P
                                                              455272-15-8P
455272-17-0P
               455272-19-2P
                               455272-21-6P
                                              455272-24-9P
                                                              455272-26-1P
455272-28-3P
               455272-29-4P
                               455278-75-8P
                                              455278-76-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
```

(Uses)

(target compd.; prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD RE

- (1) Bayer Corporation; WO 9932463 Al 1999 HCAPLUS
- (2) Saji; US 5532372 A 1996 HCAPLUS
- (3) Sekut; US 6054487 A 2000 HCAPLUS
- IT **50432-01-4**, 2,6-Diphenyl-4-aminophenol

RL: CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial study); RACT (Reactant or reagent)

(prepn. of substituted fused cyclic isoindolediones as modulators of nuclear hormone receptor function)

RN 50432-01-4 HCAPLUS

CN [1,1':3',1''-Terphenyl]-2'-ol, 5'-amino- (9CI) (CA INDEX NAME)

L8 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2003 ACS on STN

AN 2002:9831 HCAPLUS

DN 136:74279

TI Oxidative hair dye containing 2,4-diamino-1-(2-methoxyethoxy)benzene as coupler

IN Braun, Hans-Juergen; Umbricht, Gisela

PA Wella Aktiengesellschaft, Germany

SO Eur. Pat. Appl., 14 pp. CODEN: EPXXDW

DT Patent

LA German

IC ICM A61K007-13

CC 62-3 (Essential Oils and Cosmetics)

Section cross-reference(s): 25

FAN.CNT 1

FAN.	N.I. T				
	PATENT NO. KIND DATE APPLICATION NO. DATE				
ΡI	EP 1166749 A2 20020102 EP 2001-106293 20010315	20010315			
	EP 1166749 A3 20030514				
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, M	1C, PT,			
	IE, SI, LT, LV, FI, RO				
	DE 10032135 A1 20020117 DE 2000-10032135 20000701	20000701			
	JP 2002060328 A2 20020226 JP 2001-184445 20010619				
PRAI	DE 2000-10032135 A 20000701				
os	MARPAT 136:74279				
GI					

Ι

The invention concerns oxidative hair dyes that contain 2,4-diamino-1-(2-methoxyethoxy) benzene as coupler, a p-phenylene diamine deriv. (I), a 4,5-diamino-1H-pyrazole deriv. (II), and p-aminophenyl derivs. (III). Thus 2,4-diamino-1-(2-methoxyethoxy) benzene dihydrochloride was synthesized. 0.67 G of the product was used as coupler in a hair dye soln. that further contained (g): ethanol 10.0; sodium lauryl ether sulfate (28% aq. soln.) 10.0; ammonia (25% aq. soln.) 10.0; ascorbic acid 0.30; 2-hydroxymethyl-p-phenylene diamine 0.35; water to 100.

ST oxidative hair dye diaminomethoxyethoxybenzene deriv

IT Oxidizing agents

Temperature

рН

ΙT

IT

(oxidative hair dye contg. 2,4-diamino-1-(2-methoxyethoxy)benzene as coupler)

derivs. 123-30-8D, p-Aminophenol, derivs. 2835-99-6, 3-Methyl-4-aminophenol 106-50-3D, p-Phenylenediamine, derivs. 288-13-1D, Pyrazole, derivs. 19434-42-5 45514-38-3, 4,5-Diamino-1-methyl-1H-pyrazole 79352-72-0, 2-Aminomethyl-4-aminophenol 73793-79-0 73793-80-3 104333-09-7, 2-Hydroxymethyl-4-aminophenol 96886-30-5 93841-24-8 109942-17-8, [1,1'-Biphenyl]-2,5-diamine 126335-43-1 131311-66-5 155601-16-4, 4,5-Diamino-1-(1-methylethyl)-1H-132026-22-3 132026-42-7 155601-17-5, 4,5-Diamino-1-(2-hydroxyethyl)-1H-pyrazole 157469-54-0, 4,5-Diamino-1-[(4-methylphenyl)methyl]-1H-pyrazole 168202-61-7, 3-Hydroxymethyl-4-aminophenol 220264-58-4 232284-09-2 244104-61-8 246244-41-7 306959-12-6 329320-36-7 337906-36-2 349649-41-8 349649-42-9 349649-44-1 RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses) (oxidative hair dye contg. 2,4-diamino-1-(2methoxyethoxy)benzene as coupler)

methoxyethoxy; benzene as coupler;
71077-37-7P, 1,3-Diamino-4-(2-methoxyethoxy)benzene
RL: COS (Cosmetic use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(oxidative hair dye contg. 2,4-diamino-1-(2methoxyethoxy) benzene as coupler) IT 66422-98-8P RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (oxidative hair dye contq. 2,4-diamino-1-(2methoxyethoxy)benzene as coupler) IT 97-00-7, 1-Chloro-2,4-dinitrobenzene RL: RCT (Reactant); RACT (Reactant or reagent) (oxidative hair dye contg. 2,4-diamino-1-(2methoxyethoxy) benzene as coupler) IT 19434-42-5 RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses) (oxidative hair dye contg. 2,4-diamino-1-(2methoxyethoxy)benzene as coupler) 19434-42-5 HCAPLUS RN [1,1'-Biphenyl]-2-ol, 5-amino- (9CI) CN(CA INDEX NAME) Ph L8 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2003 ACS on STN 2001:903370 HCAPLUS AN DN 136:42512 TI 2-Hydroxy-5-aminobiphenyl derivatives for oxidation hair dyeing applicants compositions ΙN Chassot, Laurent; Braun, Hans-Juergen Wella A.-G., Germany PA Ger., 22 pp. SO CODEN: GWXXAW DTPatent LA German IC ICM C07C215-76 ICS A61K007-13; C07C217-84 62-3 (Essential Oils and Cosmetics) Section cross-reference(s): 25, 41 FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE PΤ DE 10032134 C1 20011213 DE 2000-10032134 20000701 WO 2002002507 20020110 A1 WO 2001-EP2704 20010310 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,

YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

20020514

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,

BR 2001-6932

20010310

BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

Α

BR 2001006932

```
20010310
    EP 1208077
                            20020529
                                           EP 2001-936066
                       Α1
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
    US 2002166180
                                           US 2002-49346
                                                             20020130
                       A1
                            20021114
PRAI DE 2000-10032134 A
                            20000701
    WO 2001-EP2704
                            20010310
    MARPAT 136:42512
OS
AΒ
    Compns. for the oxidative dyeing of hair fibers are based on a
     developer/coupling substance combination. The developer can be selected
     from 2-hydroxy-5-aminobiphenyl derivs. Thus, 2-hydroxy-5-aminobiphenyl-
    HCl (I) was prepd. by the bromination of 4-nitrophenol followed by the
     reaction with chloromethyl Me ether of the resulting bromo compd, coupling
    with phenylboronic acid in the presence of tetrakis(triphenylphosphine)pal
     ladium and catalytic redn. Thus, a hair dye formulation
     contained I 1.25 and 1,3-dihydroxybenzene (coupler) 1.25 mmol, 8% aq.
    potassium oleate soln. 1.0, 22% aq. soln. of NH3 1.0, EtOH 1.0, ascorbic
     acid 0.3, and water to 100.0 g.
     hydroxyaminobiphenyl oxidn hair dye prepn; biphenyl amino oxidn
ST
    hair dye prepn
ΙT
     Dyes
        (direct; hydroxyaminobiphenyl derivs. for oxidn. hair dyeing
        compns.)
     Hair preparations
IT
        (dyes, oxidative; hydroxyaminobiphenyl derivs. for oxidn. hair
        dyeing compns.)
IT
     Hair preparations
        (dyes; hydroxyaminobiphenyl derivs. for oxidn. hair dyeing
IT
     90-15-3, 1-Naphthol
                           95-88-5, 1-Chloro-2, 4-dihydroxybenzene
                                                                     106-50-3,
     1,4-Diaminobenzene, biological studies
                                             108-45-2, 1,3-Diaminobenzene,
     biological studies 108-46-3, 1,3-Dihydroxybenzene, biological studies
                             533-31-3, 1,3-Benzodioxol-5-ol
     123-30-8, 4-Aminophenol
                                                                 591-27-5,
     3-Aminophenol
                     608-25-3, 2-Methyl-1,3-dihydroxybenzene
                                                                615-50-9,
     2,5-Diaminotoluene sulfate 2835-95-2, 5-Amino-2-methylphenol
     2835-98-5, 2-Amino-5-methylphenol 2835-99-6, 3-Methyl-4-aminophenol
                                               6358-09-4, 2-Amino-6-chloro-4-
     5697-02-9, 1-Acetoxy-2-methylnaphthalene
                   26455-21-0, N-(3-Dimethylamino)phenylurea
     nitrophenol
                                                              28365-08-4
                              83763-48-8 84540-50-1, 3-Amino-2-chloro-6-
     63886-75-9
                  70643-20-8
                    90817-34-8, 3-Amino-2-methylamino-6-methoxypyridine
     methylphenol
                              131657-78-8, 6-Chloro-2-ethylamino-4-nitrophenol
     93841-25-9
                  94158-14-2
     135043-64-0, 4-Amino-2-aminomethylphenol dihydrochloride 155601-30-2
     169381-75-3
                   217311-43-8, 2,4-Diamino-5-fluorotoluene sulfate
                   350482-02-9
                                 379220-23-2
     350482-01-8
     RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
        (hydroxyaminobiphenyl derivs. for oxidn. hair dyeing compns.)
IT
     19434-42-5P 42961-77-3P 379219-69-9P
     379219-70-2P 379219-71-3P 379219-72-4P
     379219-73-5P 379219-74-6P 379219-75-7P
     379219-76-8P 379219-77-9P 379219-78-0P
     379219-79-1P 379219-80-4P 379219-81-5P
     379219-82-6P 379219-83-7P 379219-84-8P
     379219-85-9P 379219-86-0P 379219-87-1P
     379219-88-2P 379219-89-3P 379219-90-6P
     379219-91-7P 379219-92-8P 379219-93-9P
     379219-94-0P 379219-95-1P 379219-96-2P
     379219-97-3P 379219-98-4P 379219-99-5P
     379220-00-5P 379220-02-7P 379220-04-9P
     379220-06-1P 379220-08-3P 379220-09-4P
```

```
379220-11-8P 379220-13-0P 379220-15-2P
     379220-17-4P 379220-25-4P 379220-26-5P
     379220-27-6P 379220-28-7P 379220-29-8P
    RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation); USES (Uses)
        (hydroxyaminobiphenyl derivs. for oxidn. hair dyeing compns.)
    70-11-1, 2-Bromoacetophenone 95-46-5, 2-Bromotoluene
                                                             100-02-7,
ΙT
                                          104-95-0 106-38-7, 4-Bromotoluene
     4-Nitrophenol, reactions 104-92-7
                                                         107-30-2,
                               106-41-2, 4-Bromophenol
     106-40-1, 4-Bromoaniline
                               402-43-7 460-00-4, 1-Bromo-4-fluorobenzene
     Chloromethylmethylether
                                                 583-70-0
                                                            583-71-1
                                                                     588-96-5
                           576-23-8
                                     578-57-4
     553-94-6
               556-96-7
     591-17-3, 3-Bromotoluene
                                591-20-8, 3-Bromophenol
                                                          623-00-7,
                           1072-85-1, 1-Bromo-2-fluorobenzene
                                                                1073-06-9,
     4-Bromobenzonitrile
     1-Bromo-3-fluorobenzene
                               1422-53-3, 2-Bromo-4-fluorotoluene
     1-Bromo-4-ethylbenzene
                              1973-22-4, 1-Bromo-2-ethylbenzene
                                                                  2398-37-0
     2635-13-4, 4-Bromo-1,2-methylenedioxybenzene
                                                   2655-84-7,
                               3188-13-4, Chloromethylethylether
                                                                   3972-65-4
     1-Bromo-3-ethoxybenzene
                             6952-59-6, 3-Bromobenzonitrile
     4654-39-1
                5391-88-8
                                                             10075-50-0,
                    10269-01-9, 3-Bromo-benzylamine
                                                       14472-14-1,
     5-Bromoindole
     4-Bromo-3-methylphenol
                              17715-69-4
                                           19614-16-5
                                                      25015-63-8,
                    27060-75-9, 2-Bromo-5-methoxytoluene
                                                            34743-88-9
     Pinacolborane
     41252-83-9, 2-(2-Bromophenyl)ethanol
                                           54840-15-2
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (hydroxyaminobiphenyl derivs. for oxidn. hair dyeing compns.)
     4291-29-6P, 2-Hydroxy-5-nitrobiphenyl 5847-59-6P, 2-Bromo-4-nitrophenol
IT
                    364599-00-8P
                                   365533-48-8P
                                                  373380-62-2P
     364598-99-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (hydroxyaminobiphenyl derivs. for oxidn. hair dyeing compns.)
              THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD .
RE.CNT
RE
(1) Anon; HCAPLUS
(2) Anon; EP 0027679 A HCAPLUS
(3) Anon; EP 0873745 A2 HCAPLUS
(4) Anon; DE 2518393 A1 HCAPLUS
(5) Anon; DE 2659056 A1 HCAPLUS
     19434-42-5P 42961-77-3P 379219-69-9P
     379219-70-2P 379219-71-3P 379219-72-4P
     379219-73-5P 379219-74-6P 379219-75-7P
     379219-76-8P 379219-77-9P 379219-78-0P
     379219-79-1P 379219-80-4P 379219-81-5P
     379219-82-6P 379219-83-7P 379219-84-8P
     379219-85-9P 379219-86-0P 379219-87-1P
     379219-88-2P 379219-89-3P 379219-90-6P
     379219-91-7P 379219-92-8P 379219-93-9P
     379219-94-0P 379219-95-1P 379219-96-2P
     379219-97-3P 379219-98-4P 379219-99-5P
     379220-00-5P 379220-02-7P 379220-04-9P
     379220-06-1P 379220-08-3P 379220-09-4P
     379220-11-8P 379220-13-0P 379220-15-2P
     379220-17-4P 379220-25-4P 379220-26-5P
     379220-27-6P 379220-28-7P 379220-29-8P
     RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation); USES (Uses)
        (hydroxyaminobiphenyl derivs. for oxidn. hair dyeing compns.)
RN
     19434-42-5 HCAPLUS
CN
     [1,1'-Biphenyl]-2-ol, 5-amino- (9CI) (CA INDEX NAME)
```

RN 42961-77-3 HCAPLUS CN [1,1'-Biphenyl]-2-ol, 5-amino-, hydrochloride (9CI) (CA INDEX NAME)

HCl

RN 379219-69-9 HCAPLUS CN [1,1'-Biphenyl]-2-ol, 5-amino-2'-methyl-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 379219-70-2 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-3'-methyl-, hydrochloride (9CI) (CA INDEX NAME)

2,1

<u>ن</u>

● HCl

RN 379219-71-3 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-4'-methyl-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 379219-72-4 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 4',5-diamino-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 379219-73-5 HCAPLUS
CN [1,1'-Biphenyl]-2,4'-diol, 5-amino-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 379219-74-6 HCAPLUS CN [1,1'-Biphenyl]-2,3'-diol, 5-amino-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 379219-75-7 HCAPLUS CN [1,1'-Biphenyl]-2-ol, 5-amino-4'-fluoro-, hydrochloride (9CI) (CA INDEX NAME)

HCl

RN 379219-76-8 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-2'-fluoro-, hydrochloride (9CI) (CA INDEX NAME)

RN 379219-77-9 HCAPLUS
CN [1,1'-Biphenyl]-4-carbonitrile, 5'-amino-2'-hydroxy-, monohydrochloride
(9CI) (CA INDEX NAME)

● HCl

RN 379219-78-0 HCAPLUS
CN [1,1'-Biphenyl]-3-carbonitrile, 5'-amino-2'-hydroxy-, monohydrochloride
(9CI) (CA INDEX NAME)

● HCl

RN 379219-79-1 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-2'-ethyl-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 379219-80-4 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-4'-ethyl-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 379219-81-5 HCAPLUS CN [1,1'-Biphenyl]-2-ol, 5-amino-2',4'-diethyl-, hydrochloride (9CI) (CA INDEX NAME)

HCl

RN 379219-82-6 HCAPLUS CN [1,1'-Biphenyl]-2-ol, 5-amino-2',3'-dimethyl-, hydrochloride (9CI) (CA INDEX NAME) ELHILO 10/049346

8/28/03

Page 22

CN

RN

[1,1'-Biphenyl]-2-ol, 5-amino-2',5'-dimethyl-, hydrochloride (9CI) (CA 379219-83-7 HCAPLUS

INDEX NAME)

[1,1'-Biphenyl]-2-ol, 5-amino-3',5'-dimethyl-, hydrochloride (9CI) (CA ● HCl RNCN

INDEX NAME)

5/9219-83-9 HUAPLUS
[1,1'-Biphenyl]-2-ol, 5-amino-3'-(aminomethyl)-, monohydrochloride (9CI) HCl 379219-85-9 HCAPLUS RNCN

(CA INDEX NAME)

● HCl

RN 379219-86-0 HCAPLUS CN [1,1'-Biphenyl]-2-ol, 5-amino-4'-methoxy-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 379219-87-1 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-2'-methoxy-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 379219-88-2 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-3'-methoxy-, hydrochloride (9CI) (CA INDEX NAME)

1

HCl

RN 379219-89-3 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-5'-fluoro-2'-methyl-, hydrochloride (9CI)
(CA INDEX NAME)

• HCl

RN 379219-90-6 HCAPLUS
CN Phenol, 4-amino-2-(1H-indol-5-yl)-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 379219-91-7 HCAPLUS
CN Ethanone, 1-(5'-amino-2'-hydroxy[1,1'-biphenyl]-3-yl)-, hydrochloride
(9CI) (CA INDEX NAME)

● HCl

RN 379219-92-8 HCAPLUS
CN Phenol, 4-amino-2-(1,3-benzodioxol-5-yl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 379219-93-9 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-3'-ethoxy-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 379219-94-0 HCAPLUS CN [1,1'-Biphenyl]-2-ol, 5-amino-4'-methoxy-2'-methyl-, hydrochloride (9CI) (CA INDEX NAME)

HCl

RN 379219-95-1 HCAPLUS
CN [1,1'-Biphenyl]-2-ethanol, 5'-amino-2'-hydroxy-, hydrochloride (9CI) (CA INDEX NAME)

HCl

RN 379219-96-2 HCAPLUS CN [1,1'-Biphenyl]-2-ol, 5-amino-4'-nitro-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 379219-97-3 HCAPLUS CN [1,1'-Biphenyl]-2-ol, 5-amino-4'-(methylthio)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 379219-98-4 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-4'-(1,1-dimethylethyl)-, hydrochloride (9CI)
(CA INDEX NAME)

● HCl

RN 379219-99-5 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-2',4'-dimethoxy-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 379220-00-5 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-2',5'-dimethoxy-, hydrochloride (9CI) (CAINDEX NAME)

HCl

RN 379220-02-7 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-4'-(2-hydroxyethoxy)-, hydrochloride (9CI)
(CA INDEX NAME)

$$\begin{array}{c} \text{OH} \\ \\ \text{O-} \text{ CH}_2\text{--} \text{ CH}_2\text{--} \text{ OH} \\ \\ \\ \text{NH}_2 \end{array}$$

● HCl

RN 379220-04-9 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-4'-(trifluoromethyl)-, hydrochloride (9CI)
(CA INDEX NAME)

● HCl

RN 379220-06-1 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-3',4'-dimethyl-, hydrochloride (9CI) (CAINDEX NAME)



RN 379220-08-3 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-4'-ethoxy-, hydrochloride (9CI) (CA INDEX NAME)

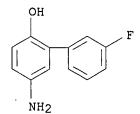
Page 29

HCl

RN 379220-09-4 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-2'-(methylthio)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 379220-11-8 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 5-amino-3'-fluoro-, hydrochloride (9CI) (CA INDEX NAME)



RN379220-13-0 HCAPLUS CN [1,1'-Biphenyl]-2,4'-diol, 5-amino-2'-methyl-, hydrochloride (9CI) (CA INDEX NAME)

HCl

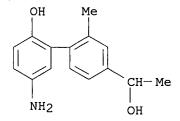
RN379220-15-2 HCAPLUS CN [1,1'-Biphenyl]-4-ethanol, 5'-amino-2'-hydroxy-2-methyl-, hydrochloride (9CI) (CA INDEX NAME)

OH Me
$$CH_2-CH_2-OH$$

$$NH_2$$

● HCl

RN379220-17-4 HCAPLUS [1,1'-Biphenyl]-4-methanol, 5'-amino-2'-hydroxy-.alpha.,2-dimethyl-, CN hydrochloride (9CI) (CA INDEX NAME)



RN 379220-25-4 HCAPLUS CN [1,1'-Biphenyl]-2,4'-diol, 5-amino- (9CI) (CA INDEX NAME)

RN 379220-26-5 HCAPLUS CN [1,1'-Biphenyl]-2-ol, 5-amino-4'-(2-hydroxyethoxy)- (9CI) (CA INDEX NAME)

RN 379220-27-6 HCAPLUS CN [1,1'-Biphenyl]-2,4'-diol, 5-amino-2'-methyl- (9CI) (CA INDEX NAME)

RN 379220-28-7 HCAPLUS

ELHILO 10/049346 8/28/03

[1,1'-Biphenyl]-4-ethanol, 5'-amino-2'-hydroxy- (9CI) (CA INDEX NAME) CN

Page 32

RN379220-29-8 HCAPLUS CN [1,1'-Biphenyl]-2-ol, 4',5-diamino- (9CI) (CA INDEX NAME)

ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2003 ACS on STN rs

2001:594358 HCAPLUS AN

135:185186 DN

ΤI Hair dye formulations containing 1-(3'-aminopropoxy)-2,4diaminobenzene and developers

Wella A.-g., Germany PA

Ger. Gebrauchsmusterschrift, 29 pp. SO

CODEN: GGXXFR

DTPatent

LA German

ICM A61K007-13 IC

62-3 (Essential Oils and Cosmetics) CC

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. ____ DE 20107481 U1 20010816 DE 2001-20107481 20010502 PΙ PRAI DE 2001-20107481 20010502

OS MARPAT 135:185186

Hair dye formulations contain a developer and coupler. AB combination. The coupler substance can be 1-(3'-aminopropoxy)-2,4diaminobenzene and/or its salt, and the developer is selected from compds. such as a p-phenylenediamine, a 4,5-diamino-1H-pyrazole, or a 4-aminophenol. Thus, 1-(3'-aminopropoxy)-2,4-diaminobenzene-3HCl was prepd. by the redn. of N-[2-(3'-aminopropoxy)-5-nitrophenyl]acetamide in the presence of palladium-charcoal and acidification with HCl. A hair dye formulation contained the above compd. 0.77, EtOH 10.00, 28% soln. of Na lauryl ether sulfate 10.00, 25% ag. soln. of NH3 10.00, ascorbic acid 0.30, 3-methyl-4-aminophenol 0.31 (developer) and water to 100 g. The formulation imparted a purple-red color to the hair.

aminopropoxydiaminobenzene hair dye developer; diaminobenzene ST

aminopropoxy hair dye developer; aminobenzene aminopropoxy hair dye developer Phenols, biological studies IT RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses) (amino; hair dye formulations contg. aminopropoxydiaminobenzene and developers) ΙT Amines, biological studies RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses) (diamines, arom.; hair dye formulations contg. aminopropoxydiaminobenzene and developers) IT Hair preparations (dyes; hair dye formulations contg. aminopropoxydiaminobenzene and developers) IT Phenols, biological studies RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses) (hair dye formulations contg. aminopropoxydiaminobenzene and developers) IT Amines, biological studies RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses) (phenolic; hair dye formulations contg. aminopropoxydiaminobenzene and developers) 100-01-6, biological studies IT 90-15-3, 1-Naphthalenol 95-88-5 123-30-8 108-46-3, 1,3-Benzenediol, biological studies 533-31-3, 1004-74-6, 1,3-Benzodioxol-5-ol 591-27-5 608-25-3 615-50-9 Pyrimidinetetramine 2835-95-2 2835~96-3 2835-98-5 2835-99-6 5392-28-9 5697-02-9 6358-09-4 **19434-42-5** 20055-01-0 26455-21-0 28365-08-4 45514-38-3 54381-16-7 70643-20-8 73793-79-0 73793-80-3 79352-72-0 81329-90-0 83732-72-3 84540-50-1 93841-24-8 .93841-25-9 96886-30-5 104333-09-7 109942-17-8, [1,1'-Biphenyl]-2,5-diamine 126335-43-1 131311-66-5 131657-78-8 132026-22-3 132026-42-7 155601-16-4 155601-17-5 157469-54-0 155601-30-2 157469-73-3 168202-61-7 173994-78-0 217311-43-8 220264-58-4 232284-09-2 244104-61-8 244104-62-9 246244-41-7 306959-12-6 329320-36-7 337906-36-2 337906-38-4 349649-41-8 344904-47-8 349649-42-9 349649-43-0 349649-44-1 .349649-46-3 354762-87-1 354762-88-2 354807-04-8 RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses) (hair dye formulations contg. aminopropoxydiaminobenzene and developers) IT 76214-09-0P RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (hair dye formulations contg. aminopropoxydiaminobenzene and developers) IT 76214-07-8 RL: RCT (Reactant); RACT (Reactant or reagent) (hair dye formulations contg. aminopropoxydiaminobenzene and developers) IT 19434-42-5 RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (hair dye formulations contg. aminopropoxydiaminobenzene and developers)